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Numerical Simulations of Detonations in Heterogeneous Explosives

Background

The work is concerned with the numerical simulation of two-phase, chemically active, granular energetic materials under compliant confinement. Due to the micro-structural complexity of these materials no *ab-initio* modelling is possible yet. Therefore granularity and its fine-scale effects on the flow are averaged out and the micro-structural effects of heterogeneity are taken into account through sub-grid-scale models. We are testing and implementing many different mathematical formulations and sub-grid-scale models. The results presented in this poster have been generated by the chemically-active Euler equations, complemented by a version of the Ignition & Growth model, which is augmented by desensitisation terms. Additional conservation laws (coupled to this system), account for the compliant confinement effects.

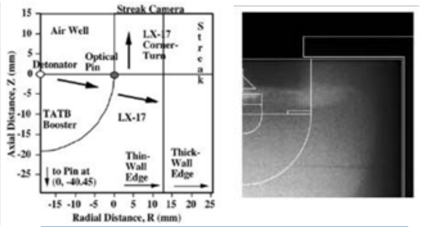

Figure 1: LX-17 Corner-Turning schematic representation and X-Ray picture, Souers et al, Propellants, Explosives, Pyrotechnics 29 (2004), No. 6

The hockey-puck experiment (shown to the left) and the challenges that it poses to numerical simulations (e.g. the existence of dead zones and the compliancy of the confiner) is representative of the problems that we wish to solve.

Mathematical Formulation and Numerical Method

The governing equations in two space dimensions are given by:

$$\mathbf{u_t} + \mathbf{f(u)_x} + \mathbf{g(u)_y} = \mathbf{h(u)},$$

where the vector **u**, the flux vectors **f (u), g(u)** and the source term **h(u)** are given by:

$$\mathbf{u} = \begin{pmatrix} \rho \\ \rho u \\ \rho w \\ \rho e \\ \rho \mu \\ \rho \lambda \end{pmatrix}, \mathbf{f(u)} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u w \\ u(\rho e + p) \\ \rho u \mu \\ \rho u \lambda \end{pmatrix}, \mathbf{g(u)} = \begin{pmatrix} \rho w \\ \rho w u \\ \rho w^2 + p \\ w(\rho e + p) \\ \rho w \mu \\ \rho w \lambda \end{pmatrix}, \mathbf{h(u)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \rho R \end{pmatrix}.$$

The first four equations are the mass, momentum and energy conservation laws. The equations for μ and λ account for the compliant confiner and species conservation respectively. The different materials are connected through a pressure p_k and temperature T_k equilibrium condition. The system of equations is closed with a set of mixture rules for the internal energy and specific volume:

$$\begin{aligned} e &= \mu\,(1-\lambda)\,e_s(p_s, v_s) + \mu\,\lambda\,e_g(p_g, v_g) + (1-\mu)\,e_i(p_i, v_i), \\ v &= \mu\,(1-\lambda)\,v_s + \mu\,\lambda\,v_g + (1-\mu)\,v_i. \end{aligned}$$

Different Jones-Wilkins-Lee (JWL) equation of states are used for each constituent, which can be expressed in mechanical and thermal Mie-Grüneisen Form:

$$\begin{aligned} e_k(p, v_k) &= e_{k,ref}(v_k) + \frac{v_k}{w_k}\left(p - p_{k,ref}(v_k)\right), \\ e_k(v_k, T) &= C_{k,V} T + e_{k,ref}(v_k), \\ p_k(v_k, T) &= \frac{w_k}{v_k} C_{k,V} T + p_{k,ref}(v_k), \end{aligned}$$

here w_k represents the Grüneisen Gamma and p_{ref} (v_k), e_{ref} (v_k) the isentropic reference curve for pressure and energy.
This system is solved numerically by means of a Riemann problem based method and it is implemented in a dynamically-adaptive mesh refinement (AMR) algorithm.

Results

A detonation wave propagating in a compliantly-confined PBX9502 rate stick is shown in figure 2. Comparison with experimental results and shock-polar analysis reveals that the correct non-ideal detonation speed and shock deflection angles have been predicted.

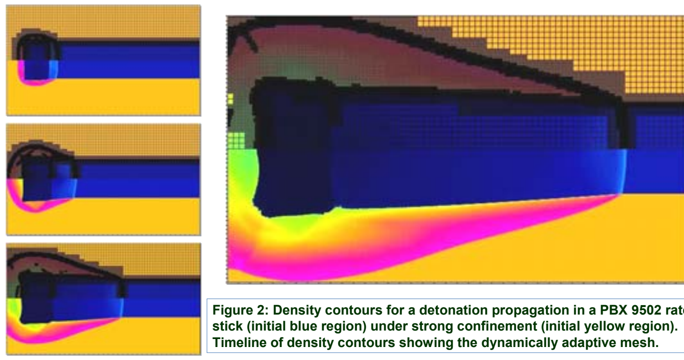

Figure 2: Density contours for a detonation propagation in a PBX 9502 rate stick (initial blue region) under strong confinement (initial yellow region). Timeline of density contours showing the dynamically adaptive mesh.

The corner turning rib (Lyle) test studies the propagation of a detonation in a curved compliantly-confined domain. Results for this problem are shown in in figure 3; the differences between simple decay theory and simulation is demonstrated in figure 4. It is found that the differences are more pronounced for bigger radii and diameters where the decay theory fails to explain the wave-speed structure.

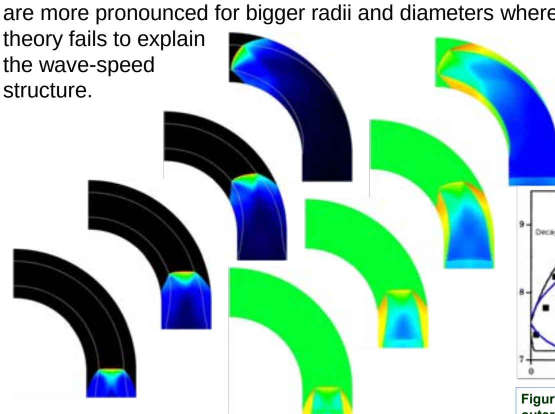

Figure 3: Numerical results (pressure and density) for the corner turning rib test (Lyle) experiment at times t = 3.5, 7.5, 11.5 and 22.5 μs after entering the curved part. The white line marks the boundary between the explosive and the confiner.

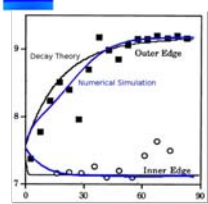

Figure 4: Measured inner and outer wave speed in [km/s] against turning angle, compared to results obtained with simple decay theory and this numerical simulation.

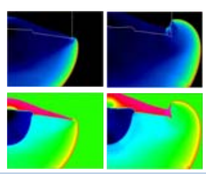

Figure 5a: Two time instances from the hockey-puck simulation, using the original model, showing density (green background) and pressure (blue). The white line marks the boundary between the explosive and the confiner.

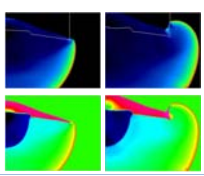

Figure 5b: As above, but using the modified (desensitised) formulation. The effect of desensitising is apparent near the apex of the corner.

The compliantly-confined hockey-puck experiment. The original Ignition & Growth model does not capture regions where the explosive (due to the operational conditions) has remained unreacted. Our formulation has been extended with a desensitisation model (proposed by DeOliveira et al 2006) which measures the consolidation of the unreacted material. Depending on the compression history, hot spots cannot form anymore in weakly pre-shocked areas and the explosive becomes desensitised. This behaviour is pronounced in sharp corner-turning experiments as shown in figure 1. Results from two numerical simulations of this experiment are shown in figures 5 and 6, where the "dead zone" is successfully captured by the modified sub-grid-scale model.

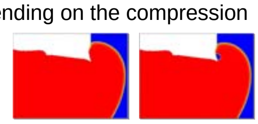

Figure 6: Contours of reaction fraction [reacted (red), unreacted (blue)] (corresponding to the final frame of figure 5) using the original (left) and the modified, desensitised model (right). The dead zone of unreacted material (blue area near the apex of the corner) is successfully captured by the modified model.

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